

Serial No. 10/699,459
Election dated April 17, 2006
In reply of Office Action dated March 16, 2006

Amendments to the Claims:

This listing of claims will replace all prior versions and listings of claims in the application.

Listing of Claims:

1(elected). A computer-based method of generating a quantitative structure activity relationship comprising:

- a) calculating a numerical representation of molecules consisting of n numbers per molecule; and,
- b) estimating a probability distribution that a said molecules is active.

2(elected). A method as recited in claim 1, wherein:

- a) said estimating step is calculated with Bayes Theorem.

3(elected).. A method as recited in claim 1, wherein:

- a) said probability distribution of said estimating step comprises n one-dimensional distributions.

Serial No. 10/699,459

Election dated April 17, 2006

In reply of Office Action dated March 16, 2006

4(withdrawn). A method as recited in claim 1, wherein:

a) said estimating step is performed by using a means to remove linear correlations between said n numbers per molecule.

5(withdrawn). A method as recited in claim 4, wherein:

a) said means to remove linear correlations between said n numbers per molecule is a principal components analysis.

6(withdrawn). A method as recited in claim 4, wherein:

a) said means to remove linear correlations between said n numbers per molecule is a matrix diagonalization.

7(withdrawn). A method as recited in claim 1, wherein:

a) said estimating step is performed by using a means to remove dependencies between said n numbers per molecule.

8(withdrawn). A method as recited in claim 7, wherein:

a) said means to remove dependencies between said n numbers per molecule is a principal components analysis.

Serial No. 10/699,459

Election dated April 17, 2006

In reply of Office Action dated March 16, 2006

9(withdrawn). A method as recited in claim 7, wherein:

a) said means to remove dependencies between said n numbers per molecule is a matrix diagonalization.

10(withdrawn). A method as recited in claim 1, wherein:

a) said estimating step is performed by estimating a distribution over a single number.

11(withdrawn). A method as recited in claim 1, wherein:

a) said estimating step is performed by replacing a single observation with a Gaussian distribution.